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A Review of material properties of $MoSe_2$ layered compound semiconductors useful for Photo electrochemical solar cells

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Abstract:
Molybdenum/tungsten dichalcogenides constitute a well-defined family of compounds which crystallize in a layer-type structure. These compounds have properties tailored for use as storage electrodes in rechargeable photoelectrochemical solar energy storage cells. These compounds find a wide range of applications in the field of catalysis and as lubricants at high temperatures and pressures. The basic structural unit of such a compound is a sandwich of three planes: one plane of transition metal atoms between two halogen atoms. The material properties of the layered semiconductors, molybdenum diselenide ($MoSe_2$). Monolayer $MoSe_2$ is a direct band gap semiconductor which has been recently investigated for low-power field effect transistors.

Keywords: *Dichalcogenide; Semiconducting Thin Film; Molybdenum Diselenide; Tungsten Diselenide; Molybdenum Tungsten Diselenide.*

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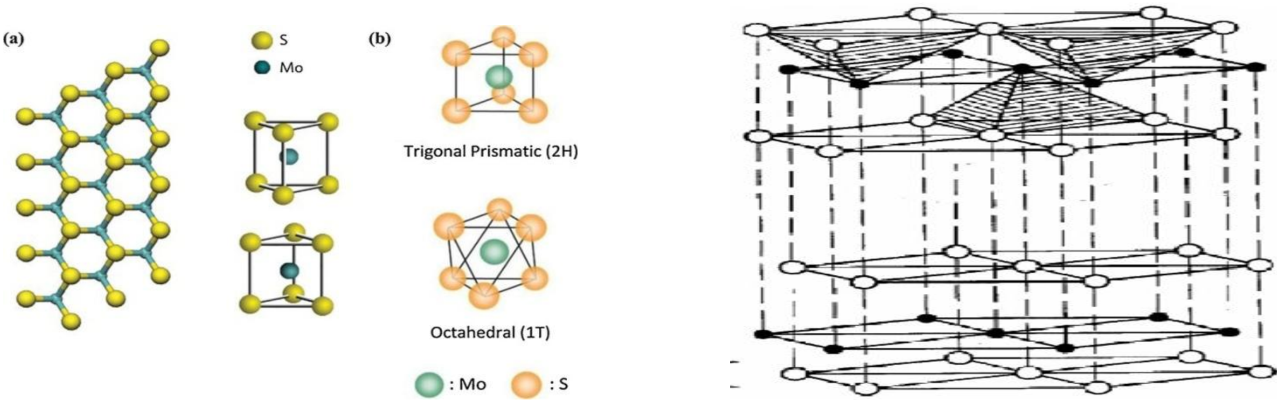
1. Introduction

As worldwide energy demands increase, conventional energy resources, such as fossil fuels, will be exhausted in the not-too-distant future. Therefore, we must develop and use alternative energy resources, especially our only long-term natural resource, the sun. The solar cell is considered as a major candidate for obtaining energy from the sun, since it can convert solar radiation directly to electricity with high conversion efficiency, it can provide nearly permanent power at low operating cost, and it is virtually free of pollution. For application in photovoltaic and photoelectrochemical (PEC) solar cells, semiconductor thin films such as CdSe, CdS, CdHgTe, GaAs, CuInSe2, CuInS, CdTe, SrTiO3, SnO2, In2O3, TiO2, SnSe, SnS, SnSSe, $MoSe_2$ and WSe2 have been elaborately studied.



(a) (b)

Figure:-1 (a) Few-layer $MoSe_2$, (b) Crystal structure showing the (hkl) planes and Mo, Se locations.

2. Methods of Preparations

There are several methods for preparing thin films. Some of them are vacuum evaporation, sputtering, hot-wall epitaxy, spray pyrolysis, chemical vapour deposition, solution growth, electrodeposition, electrode-less deposition, brush plating, screen printing, pulse electrodeposition. A simple and brief discussion about the various methods of film preparation has been discussed by Behrndt. Among molybdenum chalcogenides, $MoSe_2$ has led to the best solid-state cells with efficiencies exceeding 6%, in particular due to the surprisingly large short-circuit currents of $33 mAcm^{-2}$. based on the better performance of electrochemical cells based on $MoSe_2$ exceeding the 10% efficiency limit. The conceptional difference between a conventional hetero interface and an interface fabricated via the Vander Waals epitaxy growth good reason for hope to achieve efficiencies well above 10% after these first attempts.

3. Material properties of $MoSe_2$

1	**Type**	**p-type**
2	Structure	Hexagonal with a = 0.3285nm b = 0.3285nm c = 1.294 nm
3	Indirect band gap (eV)	Polycrystalline 1.26
4	Carrier concentration (cm^{-3})	3.3×10^{16}–7×10^{18}
5	Refractive index (n)	n_a = 4.25 (1 eV)
6	Resistivity (ohm-cm)	10^3
7	Effective mass of hole	me*≈mh*≈0.5mo (mo, free electron mass)
8	Dielectric constant (ε)	$\varepsilon_\perp$=15.4
9	Activation energy (eV)	0.08–0.57
10	Density of $MoSe_2$ ($gm\ cm^{-3}$)	6.948
11	Melting point (℃)	>1200
12	Stability	Stable

4.Result and Discussion

4.1 Surface characterization

The XRD peaks correspond to a hexagonal structure . The d-values evaluated for the dominant peaks having hexagonal structure using the JCPDS data for $MoSe_2$. The lattice parameters are calculated to be a=b= 3.210A ˚ and c = 12.592 A ˚ . From the lattice parameters and using Vegard's law, the composition of the film has been confirmed. The average grain size of these films varies in the range of 0.029–0.17 mm. The composition of the $MoSe_2$ film deposited at optimized conditions is recorded in the binding energy range from 0.00 to 20.00 keV. The intense peaks at 2.23, 1.85 and 1.70 keV confirm the elemental presence of Mo, W and Se andin the weight percentage values of 0.4077, 0.2803 and 0.0158 for $MoSe_2$, and this is shown in Figure 2.

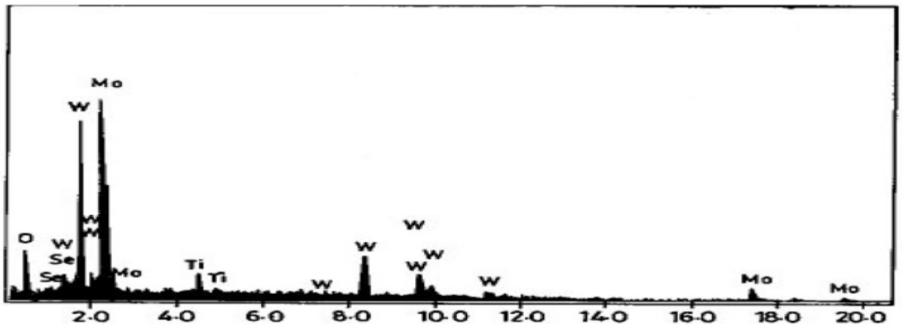


Figure-2 spectrum of $MoSe_2$ film

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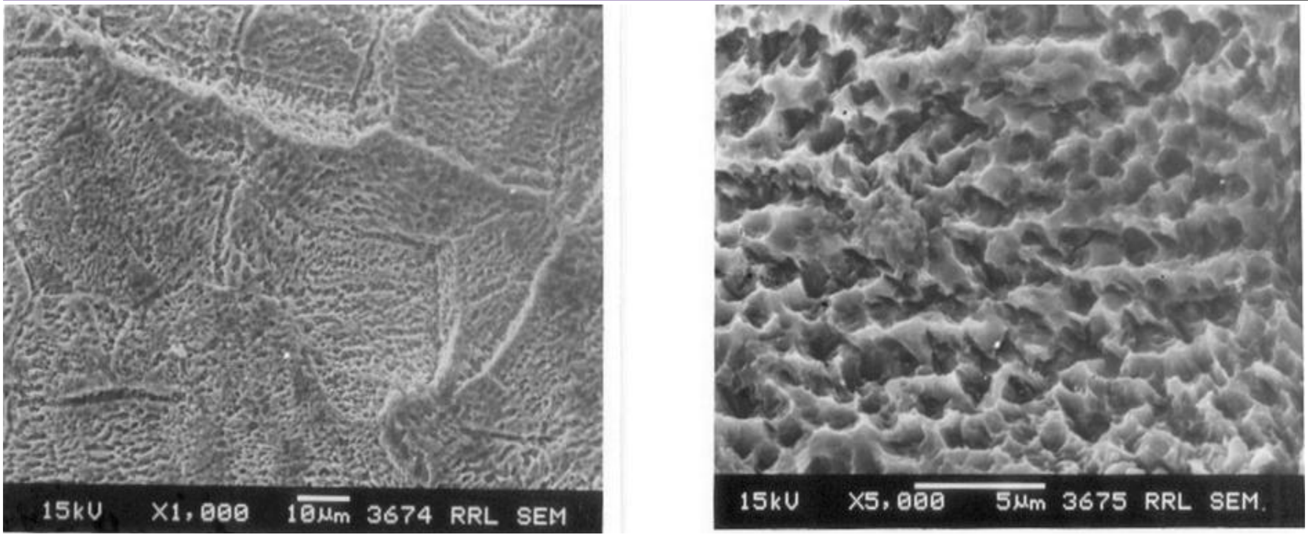

(a) (b)

Figure-3 SEM micrograph of MoSe_2 film annealed at 15°C in vacuum with magnification

4.2 SEM studies of MoSe_2

The scanning electron micrograph of an as-deposited and annealed MoSe_2 film annealed in vacuum at 150°C for 1 h deposited on a titanium substrate is shown in Figure 3(a) and (b). The grain size for the as-deposited film is 0.841 mm and for the vacuum-annealed film is 0.940 mm.

4.3 Morphology of pulse electrodeposited MoSe2 thin films

AFM images reveal that these films have a granular morphology. Irregular-shaped grains are seen. The AFM data are analysed by averaging the roughness of an area 5×5 μm^2 for various random positions on the sample surface in order to minimize the influence of local topography variation. Figure 5 shows a three-dimensional AFM image for an area of 5×5 μm^2 for MoSe_2 in the as-deposited film and annealed in vacuum at 150°C for 1 h, with a thickness of 1.0 μm. All the figures show the presence of high hills on the top of a homogeneous granular background surface. Both the density and the height of the hills increase with the thickness of the deposit. The perturbation scanned by the AFM is a measure of the crystallographic columnar size.

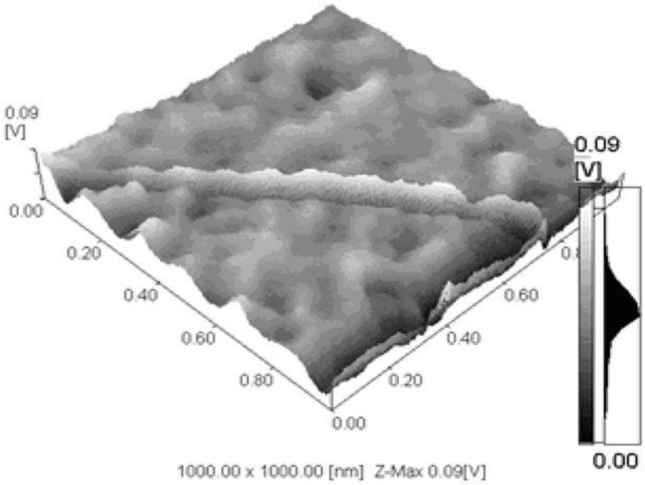

Figure-4 AFM image of MoSe_2 film

5. Conclusion

A survey on less expensive semiconducting molybdenum diselenide, tungsten diselenide and molybdenum tungsten diselenide was elaborately studied. The material properties of the films prepared using various deposition techniques are reported. The films prepared are mostly found to be polycrystalline in nature and show p- and n-type semiconducting nature. The structural, surface morphological and optical studies reveal that device quality semiconducting molybdenum / tungsten dichalcogenides can be prepared using pulse electrodeposition technique and used for PEC solar cells.

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